Green's Function Approach to B. E. Condensation in the alkali atoms

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Abstract

A new scheme has been proposed to solve the B. E. condenstates in terms of Green's function approach. It has been shown that the radial wave function of two interacting atoms, moving in a common harmonic oscillator potential modified by an effctive interaction, satisfies an intregral equation whose kernel is separable. The solution of the integral equation can be written in terms of the harmonic oscillator wave functions. The ground state wave function of the system can be written in terms of these solutions.

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The recent experimental realization of Bose-Einstein condensation [BEC] in ultra cold atomic gases has generated intensive theoretical and practical interest regarding the properties of Bose gas. Non-linear Schrodinger equation in this context known as Gross-Pitaevskii [G-P] equation [1],has been used to study the properties of the interacting spinless Bosons , trapped in harmonic potential . Altough the G-P equation is widely accepeted as a workable model for description of the B E condenstates at low temperature, the actual dynamics of B E condenstates is not fully captured by the G-P equation because of the non-integrability of the G-P equation and explicit solution is not known [2]. It is to be noted that for the positive scattering length, the G-P equation is generally solved numerically only under cylindrically symmetric systems. The Thomas Fermi approximation [3] has been introduced to get some analytical solution for the description of B E condenstates. On the other hand for the negative scattering length the G-P equation is yet to be properly investigated [3]properly. Another alternative approach to study the dynamics of the B.E.condenstates is the time dependent variation technique [4] in which one assumes fixed profile of the condenstate and computes the evolution of some parameters such as the width by variational techniques. It should also be mentioned that the negative scattering length provides stable solution of the G-P equation only under certain conditions for the number of particles and the size of the trap [5]. When those conditions are not fulfiled the condenstates become unstable. Therefore realization of large condenstates will provide reliable experimental data for the precise understanding of the condensation process[6]. In this paper we shall present a new solution for the condenstate on the basis of Green's function approach of scattering theory. Similar method was used in the treatment of the nuclear many body problems by Bethe and Goldstone; Brueckner and Gammel [7] for the understanding of the various aspects nuclear many body problem. We have derived an integral equation for the description of two interacting bosons in the presence of many bosons. We shall consider a system of N spinless interacting atoms all having the same hyperfine species, in equilibrium and at very low temperature and densities characteristic of alkali atoms under Bose-Einstein condensation (BEC) condition. We assume that each of the atoms is moving in the influence of a common harmonic oscillator potential which is called a trapping potential(V_{ext}) and an effective two-body interaction acting between them which modifies their behaviour . The essential questions we wish to investigate are : How does the effective two body interaction modify

the two-body wave function?. How does the energies of the two interacting bosons system change when the two- body effective interaction is switched on ? It is welknown that the scattering length (a_s) is very small compared to the interatomic distant(r_{int}) [8] under BEC in the dilute atomic alkali gases. Therefore the behaviour of the atoms is extremely sensitive to the details of the trap and the effective two- body interaction. Since the effective two- body interaction is very weak the quantitative calculation based on perturbation theory in the interatomic interaction is hoped to be highly reliable for the alkali gases. Furthermore the de Broglie wave length associated with individual atom is comparable to interatomic r_{int} distance therefore the correlation between atoms becomes important[7]. Hence the construction of the many -body condenstate state wave function of the system in terms of two-body wave function will be interesting. The standard many-body wave function in terms of Hartree-Fock ansatz using the single particle solution of the G-P equation does not take into accoutn the effect of correlation between atoms which is very important in the case of BEC alkali gases.In this letter we have presented an analytical formalism to investigate the above aspects of BEC problem without any numerical estimate for a particular choice of the effective interaction.That will be communicated shortly.

Let us consider a system of interacting N spinless atoms and now arbitrarily pick out any two interacting spinless atoms, say 1 and 2, denoting their relative and center-of- mass co-ordinates, by $\vec{r}$ and $\vec{R}$ respectively . We shall investigate the state (ϕ) of these two interacting atoms trapped in a common harmonic potential in the presence $(N-2)$ interacting atoms. The most general states of the many-body system will then be described by a wave function $\Psi(\vec{r},\vec{R},\chi,t)$ where χ represents schemitically the co-ordinates of the remaining $(N-2)$ particles. It is the dependence on $\vec{r}$ that is crucial but the parameter dependence of Ψ on $\vec{R},\chi$ and t will be ignored . In the present context we assume that simple BEC is realised in the two-particle state $\phi(\vec{r})$ whose equatiom of motion will be determined using Schrodinger equation. From the knowledge of the wave-function of two-atom system $\phi(\vec{r})$, the many- body ground state of B E condenstate system of alkali atoms can be written. The hamiltonian for the two- atom system in the common harmonic oscillator potential of frequency ω is given by

$$H_0 = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{m\omega^2 r_1^2}{2} + \frac{m\omega^2 r_2^2}{2}. \qquad (1)$$

Introducing the cannonical co-ordinate transform

$$\vec{r} = \vec{r}_2 - \vec{r}_1, \vec{p} = \frac{(\vec{p}_2 - \vec{p}_1)}{2}, \tag{2}$$

and

$$\vec{R} = \frac{(\vec{r}_2 + \vec{r}_1)}{2}, \vec{P} = (\vec{p}_2 + \vec{p}_1). \tag{3}$$

The hamiltonian is transformed to

$$H_0 = \frac{(P^2 + M^2\omega^2 R^2)}{2M} + \frac{(p^2 + \mu^2\omega^2 r^2)}{2\mu}, \tag{4}$$

where M=2m,$\mu = \frac{m}{2}$. The Schrodinger equation for the system with $\hbar = 1$ is

$$[\frac{(-\nabla_R^2 + M^2\omega^2 R^2)}{2M} + \frac{(-\nabla_r^2 + \mu^2\omega^2 r^2)}{2\mu}]\phi(\vec{r})\phi(\vec{R}) = E^0\phi(\vec{r})\phi(\vec{R}). \tag{5}$$

The Schrodinger equation for the relative motion is then

$$H_0\phi(\vec{r}) = (-\frac{\nabla^2}{2\mu} + kr^2)\phi(r) = E^0\phi(\vec{r}), \tag{6}$$

where

$$k = \frac{\mu\omega^2}{2} = \frac{m\omega^2}{4}. \tag{7}$$

The solutions are given by

$$\phi_{nl}^m(\vec{r}) = \frac{R_{nl}(r)}{r} Y_{lm}(\hat{r}), \tag{8}$$

where $Y_{lm}(\hat{r})$ are the usual spherical harmonics. The radial wave function $R_{nl}(r)$ is given by

$$R_{nl}(r) = N_{nl} exp(-\frac{\nu r^2}{2}) r^{l+1} v_{nl}(r), \tag{9}$$

where $\nu = \frac{\omega\mu}{\hbar}$ and $v_{nl}(r)$ is the associated Laguerre polynomial:

$$v_{nl}(r) = L_{n+l+\frac{1}{2}}^{l+\frac{1}{2}}(\nu r^2). \tag{10}$$

N_{nl} is determind by the normalization condition and $E^0_{nl} = \hbar\omega(2n + l + \frac{3}{2})$.

We shall now treat the effective spin independent two-body interaction $v(r)$ which is very weak between two atoms , as a peturbation and solve the Schrodinger equation using the Green's function method to determine the perturbed wave function for the two- atom system. The unperturbed wave function is given by

$$\phi_{nl}(\vec{r}) = \frac{R_{nl}(r)}{r} Y_{lm}(\hat{r}). \tag{11}$$

Similarly the perturbed wave function can be written as

$$\psi_{n_1 l_1}(r) = \frac{u_{n_1 l_1}}{r} Y_{l_1 m_1}(\hat{r}). \tag{12}$$

The Schrodinger equation for the perturbed system is

$$[H_0 + v(r)]\frac{u_{n_1 l_1}}{r} Y_{m_1 l_1}(\hat{r}) = E_{n_1 l_1}\frac{u_{n_1 l_1}}{r} Y_{m_1 l_1}(\hat{r}), \tag{13}$$

where $E_{n_1 l_1}$ is the perturbed energy eigen value. We now write

$$H_0\frac{R_{nl}(r)}{r} Y_{lm}(\hat{r}) = \frac{1}{r}[-\frac{1}{m}\frac{\partial^2}{\partial r^2} + V_l(r)]R_{nl}(r)Y_{nl}(\hat{r}) = E^0_{nl}\frac{R_{nl}(r)}{r} Y_{nl}(\hat{r}). \tag{14}$$

Multiplying the perturbed equation(13) by $Y^*_{n_1 l_1}(\hat{r})$ on the left and integrating over the solid angle $d\hat{r}$ we obtain

$$[E_{n_1 l_1} - (-\frac{1}{m}\frac{d^2}{dr^2} + V_{l_1}(r)]u_{n_1 l_1}(r) = v_{l_1}(r)u_{n_1 l_1}(r), \tag{15}$$

where

$$v_{l_1}(r) = \int d\vec{r} Y^*_{l_1 m_1}(\hat{r}) v(r) Y_{l_1 m_1}(\hat{r}) \tag{16}$$

In order to solve this equation we introduce Green's $G_{n_1 l'_1}(\vec{r}, \vec{r}')$ corresponding to equ.(15) satisfies the equation

$$(E_{n_1 l_1} - H_0)G_{n_1 l_1}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}'). \tag{17}$$

Multiplying through on the left by $Y^*_{l_1 m_1}(\hat{r})$ and integrate over the solid angle dr we obtain

$$[E_{n_l l_1} - (-\frac{1}{m}\frac{d^2}{dr^2}) + V_{l_1}(r)]g_{n_1 l_1}(r, r') = \delta(r - r'), \tag{18}$$

where

$$g_{n_1 l_1}(r, r') = \sum_{n_2} \frac{R_{n_2 l_1}(r) R_{n_2 l_1}(r')}{E_{n_1 l_1, n_2 l_1}}, \tag{19}$$

where

$$E_{n_1 l_1, n_2 l_2} = (E_{n_1 l_1} - E^0_{n_2 l_1}). \tag{20}$$

Hence the perturbed wave function $u_{n_1 l_1}(r)$ satisfies an integral equation with a separable kernel. Therefore we write

$$u_{n_1 l_1}(r) = \int_0^\infty dr' g_{n_1 l_1}(r, r') v_{l_1}(r') u_{n_1 l_1}(r'). \tag{21}$$

Finally we write

$$u_{n_1 l_1}(r) = \sum_{n_2=0}^{\infty} \frac{R_{n_2 l_1}(r)}{E_{n_1 l_1}, n_2 l_1} \int_0^\infty dr' R_{n_2 l_1}(r') v_{l_1}(r') u_{n_1 l_1}(r'). \tag{22}$$

The equation for $R_{n l_1}(r)$ is

$$[E^0_{n l_1} - (-\frac{1}{m}\frac{d^2}{dr^2} + V_{l1}(r))] R_{n l_1}(r) = o. \tag{23}$$

Multiplying equ.(15)and equ.(23) on the left by $R_{n l_1}(r)$ and $u_{n_1 l_1}$respectively subtracting and integrating over r' we obtain

$$E_{n_1 l_1} - E^0_{n l_1} = \frac{\int_0^\infty dr R_{n l_1}(r) v_l(r) u_{n_1 l_1}(r)}{\int_0^\infty dr R_{n l_1}(r) u_{n_1 l_1}(r)} \tag{24}$$

and the perturbed wavefunction $u_{n_1 l_1}(r)$ in a closed form can be written as

$$u_{n_1 l_1}(r) = \sum_{n_2=0}^{\infty} K_{n_1 l_1, n_2 l_1} R_{n_2 l_1}(r), \tag{25}$$

where

$$K_{n_1 l_1, n_2 l_1} = \frac{1}{E_{n_1 l_1, n_2, l_1}} \int_0^\infty dr R_{n_2 l_1}(r) v_{l_1}(r) u_{n_1 l_1}(r). \tag{26}$$

. To this expression of $u_{n_1 l_1}$ we should add the solution of $(E_{n_1 l_1} - H_0)\chi_{n_1 l_1} = 0$. Since $E_{n_1 l_1} \neq E^0_{n l_1}$ the equation $(E_{n_1, l_1} - H_0)\chi_{n_1 l_1} = 0$ has no solution.Thus

it is not necessary to add a particular solution to the $u_{n_1 l_1}$. From equations(25) and (26)it follows that

$$K_{n_1 l_1, n_2 l_1} = \frac{1}{E_{n_1 l_1, n_2 l_1}} \sum_{n_3=0}^{\infty} K_{n_1 l_1, n_3 l_1} \int_0^{\infty} dr R_{n_2 l_1}(r) v_{l_1}(r) R_{n_3 l_1}(r). \qquad (27)$$

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Results and Discussion

The main conclusions of the paper are the following: It should be noted that n_3 can in principle run from o to ∞, the above equ.(27) reprsents an infinite set of simultaneous homogeneous algebraic equations in $K_{n_1 l_1, n_2 l_1}$. The consistency of the these equations imposes the condition of vanishing of the determinant formed from the coefficients of $K_{n_1 l_1, n_2 l_1}$. This condition determines the energy shift $E_{n_1 l_1, n l_1}$of the two interacting atoms. The corresponding eigenvectors when substituted in eq.(26) determine the perturbed radial function $u_{n_1 l_1}(r)$. Since B E condensation takes place strictly in the ground state of the system therefore a few values of n_3 in the sum will provide a very reliable estimate of the two-particle wave function. Because of the separable structure of eq.(21) we can also include various types of central and non central of two-body effective interaction and the variation of the scattering length can also be incorporated to investigate sensitivity of the two-body condenstate wave function and the stability of the Bose-Einstein condensation in alkali atoms on the effective two-body interaction which can not be so easily taken care in the formalism of G-P equation. When the effective two-body interaction becomes non-central in nature then the radial equation for $u_{n_1 l_1}(r)$ i.e eq.(21) will satisfy a coupled integral equation. When the effective two-body interaction is a pseudo- potential type, as commonly used in the calculation of G-P equation, the determination of the two-body wave function $u_{n_1 l_1}(r)$ becomes extermely simple in this formalism. We can also investigate the importance two- particle correlation in BEC. Finally the construction of the condenstate wave function describing the BEC of the in terms of the calculated two- particle wave function to study various aspects of BEC becomes possible. These are the main conclusions of the paper.

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